

1. INTRODUCTION

Heavy Vehicle Propulsion Materials

Advanced materials are an enabling technology for fuel-efficient heavy-vehicle truck engines. The Heavy Vehicle Propulsion Materials Project is organized around the following technology issues: fuel systems; exhaust aftertreatment; air handling, hot section, and structural components; and standards.

Materials for Fuel Systems

Currently, the fuel system represents a significant portion of the cost of a heavy-duty diesel engine. Enabling materials and cost-effective precision manufacturing processes are instrumental in developing improved fuel injection systems. In addition to new and improved materials, improved manufacturing and inspection methods for the injector components are being developed.

Manufacturing technology for nickel aluminide–titanium carbide cermet fuel system components continued this year in coordinated efforts at Oak Ridge National Laboratory (ORNL), CoorsTek, Inc., and Cummins, Inc. ORNL supplied a large pilot-scale batch of processed powder mixtures with alternate Ni_3Al precursors to CoorsTek (a parts supplier) for injection molding of test components and completed work with CoorsTek for scale-up of the manufacturing process. Sintered parts were supplied to Cummins Engine for rig testing of machined components.

A novel “pin-on-twin” scuffing test has been developed to evaluate fuel injector materials in diesel fuel and low-sulfur fuel environments in a simulated fuel system environment. It is in beneficial use for evaluating fuel system materials. The system is available to users of the High Temperature Materials Laboratory (HTML) at ORNL, as well as to the Propulsion Materials Program.

Materials for Exhaust Aftertreatment

The reduction of nitrogen oxides (NO_x) and particulate emissions is critically important to the Office of FreedomCAR and Vehicle Technologies (OFCVT) program and is highly materials dependent. The U.S. Department of Energy (DOE) goals for improved efficiency of heavy vehicles are greatly complicated by engine design and exhaust aftertreatment technologies designed to meet the mandatory U.S. Environmental Protection Agency (EPA) emission regulations for 2007 and 2010. Materials and systems research is being conducted to minimize the potentially negative effects of emission-reduction technologies on fuel economy and to result in cleaner and more efficient engines.

The durability of exhaust aftertreatment systems in heavy vehicles is a concern. A lifetime of at least 500,000 miles is expected, and a 1,000,000-mile lifetime is desired (compared with 100,000 miles for automobiles). Exposure of the aftertreatment systems to high temperatures, vibration, erosion, and chemical attack by species in the oil and fuel results in degradation of performance. The effects of exposure in service on the microstructure and microchemistry of the aftertreatment systems are being characterized, and this research may lead to the development of more durable systems. The development of advanced NO_x sensors is being pursued to facilitate optimal engine and aftertreatment control strategies.

Accomplishments this year included significant progress in a collaborative Ford–ORNL program intended to facilitate deployment of a NO_x trap for lean diesel or gasoline exhaust by (1) investigating materials issues related to deterioration of NO_x trap performance with aging as a result of thermal and sulfation-desulfation cycles and (2) investigating materials that are robust under the lean NO_x trap operating conditions. The latter objective includes the synthesis of new materials. Accomplishments of this effort include completing a study

of microstructural changes in a series of model catalysts during aging under lean and rich conditions at 500°C; beginning the updating of the ex-situ reactor to enable transmission electron microscopy (TEM) sampling under lean, rich, or stoichiometric conditions as well as lean-rich cycles; and equipping a new synthesis laboratory for the preparation of NO_x trap materials.

A new agreement was initiated entitled “Catalyst Materials by Design.” The effort is led by a team that includes ORNL, the University of Notre Dame, and the University of California at Davis. The objective is to search for durable emissions catalysts by means of an integrated approach using computational modeling, synthesis and processing, characterization via high-resolution scanning TEM/TEM, and testing of catalyst materials. Computational modeling was carried out using density-functional-theory-based first-principles calculations. A series of platinum and rhenium (Re) nanoclusters, Re nanoclusters, and carbonylated Re clusters supported on commercial alumina were synthesized and characterized with respect to the size and chemistry of atomic clusters and the performance of the clusters in contact with carbon monoxide, NO_x, and hydrocarbons.

Research conducted at the High Temperature Materials Laboratory at ORNL is focused on the development and utilization of new capabilities and techniques for ultra-high-resolution scanning TEM/TEM to characterize the microstructures of catalytic materials of interest for reducing NO_x emissions in diesel and automotive exhaust systems. This research aims to relate the effects of reaction conditions on the changes in morphology of heavy metal species on “real” catalyst support materials, typically oxides. During this period, the morphologies of tri-rhenium carbonyl clusters on gamma-alumina support material were characterized at the atomic level to demonstrate for the first time the unambiguous imaging of clusters of known structure. Also, the nature of platinum catalyst structures on mixed-oxide support materials was characterized, including the imaging of platinum species dispersed as single atoms and in precrystalline clusters known as “rafts.”

Exhaust aftertreatment materials projects are ongoing at both Caterpillar and Cummins. These projects are significant in that they represent a departure from an earlier culture in which the diesel engine companies relied heavily on catalyst manufacturers to provide the needed technologies and did not actively participate in the development of catalyst materials. These diesel engine manufacturers are actively collaborating with catalyst suppliers in the development of improved catalyst materials, and they are contributing to the development of a fundamental understanding of catalyst performance that is important to both suppliers and users of catalyst systems. In addition to the in-house efforts at Caterpillar and Cummins, Cummins and ORNL collaborated, through cooperative research and development agreements, in characterizing lab- and engine-tested catalysts via X-ray diffraction, spectroscopy, and microscopy. They also collaborated in characterizing diesel particulate filters and developing probabilistic design tools to predict the useful lifetimes of the filters.

Ford Motor Co. and ORNL are collaborating on the development of a NO_x sensor that can be used in systems for on-board remediation of diesel engine exhaust. The sensor should have an operating temperature of 600–700°C and be able to measure NO_x concentrations from 1 to 1500 ppm at oxygen levels from 5 to 20 vol %. Prototype sensing elements are fabricated by patterning electronically conductive and catalytic layers onto oxygen-ion-conducting substrates. The sensing elements are characterized for NO_x response, oxygen sensitivity, and response time. Accomplishments this year included developing sensing elements that display near “total NO_x” behavior and are stable in simulated long-term service.

Materials for Air Handling, Hot Section, and Structural Applications

Engine design strategies for meeting EPA emission requirements have resulted in the need for significantly higher turbocharger boost. The higher boost requirements result in higher heat of compression and greater thermal and fatigue loads on turbocharger components.

Caterpillar began a new project in 2003 to design and fabricate a cost-competitive diesel engine turbocharger, using lightweight titanium materials, that provides a reduction in both fuel consumption and transient emissions. Caterpillar has designed a series turbocharger for use on the C15 engine platform. This turbocharger consists of one turbo wheel and two compressor wheels that are attached to a single rotating drive shaft. This compact design will replace the two-turbocharger system that is presently installed in the C15 engine. Titanium aluminide will be used for the turbo wheel, and one of the compressor wheels will be made from a titanium alloy. The project was completed this year. Highlights include successfully developing joining technology for the rotor and shaft, evaluating the physical and mechanical properties of commercially available materials, and accessing the commercial viability of the advanced turbocharger.

Caterpillar and ORNL won a 2003 R&D 100 Award for the development of CF8C-Plus cast stainless steel. The new high-temperature stainless steel may have near-term applications in diesel engine exhaust manifolds and turbocharger housings. Highlights include demonstrating that CF8C-Plus cast stainless steel is far superior to SiMo cast iron at 600°C and above. CF8C-Plus also shows strength, creep resistance, and aging resistance benefits compared with other commercial cast stainless steels being considered for heavy-duty diesel turbocharger housings at 750°C. Significant progress has been made in commercializing the alloy: a 6700-lb gas-turbine end-cover was cast from CF8C-Plus at MetalTek. MetalTek has cast more than 30,000 lb for various applications.

Caterpillar, in collaboration with Argonne National Laboratory and ORNL, has a project to design and fabricate prototype engine valves from silicon nitride and TiAl materials that are 30% lighter than steel valves, provide a 200% increase in service lifetime, and potentially increase fuel efficiency in advanced engines by 10%. A probabilistic design approach was developed for the high-hardness valve materials. The friction welding of TiAl valve heads and Ti-6V-4Al valve stems was successfully optimized. The effects of surface finish on the performance of silicon nitride valves were evaluated, and the results indicated that valves with good surface finish performed well in bench tests.

This year, in preparation for an engine test to be conducted in FY 2006, test valves were procured and characterized for dimensional and surface properties and via laser-scattering for surface or sub-surface defects. In addition, an evaluation of the machinability of TiAl was initiated, along with a study of friction, wear, and corrosion of the alloy. A Caterpillar C15 ACERT™ engine was donated to the National Transportation Research Center for future component testing.

Caterpillar is also developing innovative approaches to thermal barrier and wear-resistant coatings for engines. Durability issues for thermal sprayed coatings, particularly thermal barrier coatings, remain the major technical challenge to their implementation in new engine designs. New approaches to coating design and fabrication are being developed to aid in overcoming this technical hurdle. A highlight from this year is the coating of pistons for a homogeneous charge compression ignition system with amorphous steel for single-cylinder engine testing.

The feasibility of reducing the weight of a heavy-duty engine by substituting a lighter material for the cast iron engine block and cylinder head was evaluated by ORNL and Ricardo, Inc. Finite element analysis was used to compute the stresses, temperatures, and fatigue safety factors of a 5.9-L diesel engine, run at the maximum design power, for three lightweight casting alloy systems: titanium, aluminum, and magnesium. The analysis indicated the feasibility of simple material substitutions in all cases, with the exception that the titanium alloy cylinder head will require inserts to reduce the temperature in the valve bridge area. Reducing the weight of the entire engine by up to 33% for the magnesium alloy and 20% for the aluminum alloy, and up-rating the power of the engine by 50% while reducing the weight by 15% for the titanium alloy, were predicted to be feasible.

Efforts in cost-effective manufacturing were carried out by ORNL, the University of Michigan, and Purdue University. Technology for machining difficult materials, such as titanium alloys, was developed in the ORNL/University of Michigan collaboration. ORNL characterized the grinding characteristics of TiC/Ni₃Al matrix cermets that are promising candidates for diesel engine fuel injector plungers and wear parts, and investigated the possibility of using cermets as cutting tool materials for high-speed titanium machining. The University of Michigan and ORNL participated in a consortium of manufacturers led by Third Wave Systems, Inc., to develop finite-element-analysis-based machining modeling software and to acquire new machining process modeling capabilities. Purdue University is investigating the consolidation of low-cost machining chips to produce nanocrystalline components with high strength and hardness.

Materials and Testing Standards

OFCVT has an International Energy Agency “Implementing Agreement for a Programme of Research and Development on Advanced Materials for Transportation Applications.” Accomplishments this year include the development by NIST of a new design principle for surface texture design to enable friction reduction under boundary lubrication conditions.

NIST also leads a project to develop standard testing methods for advanced materials, primarily ceramics. During this year, NIST revised, refined, and improved several current ASTM and ISO standards.

The rolling contact fatigue (RCF) effort is led by ORNL. Its objectives include the characterization of the RCF performance of ceramics and tribological coatings; determination of the effects of subsurface damage, microstructure, material properties, and contact stress on RCF performance; and correlation of RCF performance measured by different internationally-used RCF test techniques. Highlights this year include completion of a summary report on RCF test methods and result interpretations used in Germany, Japan, United Kingdom, and the United States and the development of a method to evaluate and discriminate the elastic properties of ball bearings in situ using resonance ultrasound spectroscopy.

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